

Michael E. Wall

CURRICULUM VITAE

(Updated 1/29/08)

Personal Data

Citizenship: USA

Work Address: Mail Stop B256
Information Sciences Group
Computer, Computational, and Statistical Sciences Division
Los Alamos National Laboratory
Los Alamos, NM 87545

Position Team Leader

Education B.S. Physics, University of California, San Diego (1989)
Ph.D. Physics, Princeton University (1996)

Professional Experience

1996-1999	Postdoctoral Fellow, Dept of Biochemistry and Cell Biology and Keck Center for Computational Biology, Rice University
1999-2001	Postdoctoral Research Associate, Chemistry Division, Bioscience Division, and Computer and Computational Sciences Division, Los Alamos National Laboratory
2001-present	Technical Staff Member, Computer, Computational, and Statistical Sciences Division, Los Alamos National Laboratory
2001-present	Affiliate, Bioscience Division
2005-present	Team Leader, Computational Biology and Bioinformatics
2007-present	Affiliate, Center for Nonlinear Studies

Honors and Awards

Keck Center for Computational Biology NSF Postdoctoral Fellowship (1996-1998); Robert A. Welch Foundation Postdoctoral Fellowship (1996-1999); Best poster presentation, Keck Center Annual Research Conference on Computational Biology (1997)

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Service

Cultural exchange: Invited participant, 6th Annual Japanese-American Beckman Frontiers of Science Symposium, Kanagawa, Japan (Dec 2003)

Meetings: Organizer, Second q-bio Conference on Cellular Information Processing (Santa Fe, Aug 2008); Organizer, First q-bio Conference on Cellular Information Processing (Santa Fe, Aug 2007); Organizer and Lecturer, First Annual q-bio Summer School on Cellular Information Processing (Los Alamos, Jul-Aug 2007); Organizer and Speaker, Los Alamos Theory, Simulations, and Computing Capability Workshop on Computational Systems Biology (LANL, Oct 2006)

Presentations for external review committees: University of California Science & Technology Review of DOE Labs (2005); DOE Tri-Lab Review of National Security Labs (2005); and the Center for Nonlinear Studies (2005)

Referee, funding agencies and grant programs: National Institutes of Health; South Carolina Research Centers of Excellence; Army Research Office; UCR-LANL Collaborative Program; Swiss Federal Computing Center at ETH Zurich/Lausanne/Manno; LANL Laboratory-Directed Research and Development, Exploratory Research Program

Referee, journals: Nature; Physical Review Letters; Physical Review E; Physica D; Journal of Theoretical Biology; Bioinformatics; European Biophysics Journal; Biophysical Journal; Proteins; Journal of Molecular Biology; Trends in Microbiology; Nucleic Acids Research; Briefings in Bioinformatics; BMC Bioinformatics; IET Systems Biology

Professional society memberships: American Physical Society (1990-present); Biophysical Society (1992-present)

Invited Talks

Department of Computational Biology, 11/7/07, University of Pittsburgh Medical Center, Pittsburgh, PA. Invited talk: Computational studies of protein function using dynamics perturbation analysis.

Bioinformatics Research Center, 9/7/07, University of North Carolina, Charlotte, NC. Invited talk: Protein interactions and energy landscapes.

Workshop on Small-Angle X-ray Scattering in Biological Sciences, 5/31/07-6/1/07, Colorado State University, Fort Collins, CO. Invited talk: Large-scale shape changes associated with activation of cGMP-dependent protein kinase.

Department of Microbiology, University of Otago, Dunedin, New Zealand, 12/15/2006. Invited colloquium: Computational modeling of gene regulation in *Escherichia coli*.

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Second International Conference of the Biocomputing and Physics of Complex Systems Research Institute (BIFI), University of Zaragoza, Zaragoza, Spain. 8-11 February 2006. Invited talk: Principles of Biochemical Regulation. Session chair.

13th Annual International Meeting on Microbial Genomics, University of Wisconsin, Madison, WI. 11-15 September 2005. Invited talk: Computational Models of Biochemical Regulation.

International Conference on Molecular Systems Biology 2004, 8/21/04-8/25/04, Tahoe City, CA. Invited talk: Design principles of genetic regulatory networks.

Institute for Pure and applied Mathematics, 4/1/04, UCLA, Los Angeles. Invited colloquium: Structure and function of genetic regulatory circuits in *Escherichia coli*.

MIPNETS workshop on Proteins and Signals, 6/25/2003, Liverpool, UK. Invited talk: Mechanisms of Biochemical Regulation. Session chair.

University of Otago, 5/2/2003, Dunedin, New Zealand. Invited talk: Mechanisms of biochemical regulation.

American Physical Society meeting, 3/2/2003, Austin TX. Invited tutorial: Transcriptional Regulatory Networks: Data, Analysis and Modeling

LANL workshop on enabling concepts in systems biology, 9/19/2002, Santa Fe, NM. Invited talk: Integrating systems and structural biology: structural mechanisms in cGMP binding and activation of cGMP-dependent protein kinase

American Chemical Society Rocky Mountain Regional Meeting, 10/14/2002, Albuquerque, NM. Invited talk: Mechanisms associated with cGMP binding and activation of cGMP-dependent protein kinase

Instituto Gulbenkian de Ciencia, 3/11-3/15/2002, Oeiras, Portugal. Institute-sponsored visit; bioinformatics lectures on microarray methods.

APS User Meeting, 10/9/2001, Argonne National Laboratory, Argonne, IL. Invited talk: Diffuse Scattering: Methods for Molecular Structure and Dynamics

LANL/UCSD Workshop, 9/8/2001-9/9/2001, San Diego, CA. Invited talk: Diffuse Scattering and Database Methods

National Center for Genome Resources, March 2001, Santa Fe, NM. Invited seminar: Singular value decomposition analysis of microarray data

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Gordon Research Conference on Diffraction Methods in Molecular Biology, Summer 2000, Andover, NH. Invited talk: Harnessing the potential of a structure database

Los Alamos National Laboratory, February 1999, Los Alamos, NM. Invited talk: Refinement of X-ray structures using a database of pairwise interatomic distance probabilities

School of Biological Sciences, December 1998, Auckland University, Auckland, New Zealand. Invited talk: Dynamics in Calmodulin

Department of Chemistry, December 1998, Massey University, Palmerston North, New Zealand. Invited talk: Dynamics in Calmodulin

Department of Biochemistry, December 1998, Otago University, Dunedin, New Zealand. Invited talk: Dynamics in Calmodulin

Gordon Research Conference on Diffraction Methods in Molecular Biology, Summer 1998, Andover, NH. Invited talk: Making sense of diffuse scattering and making use of all the X-rays

Parke-Davis Pharmaceuticals, Spring 1998, Ann Arbor, MI. Two invited talks: Dynamics in calmodulin crystals; Refinement of X-ray structures using a database of pairwise interatomic distance probabilities

Biophysical Society Meeting, Winter 1998, Kansas City, MO. Invited talk: Refinement of X-ray structures using a database of pairwise atomic distance probabilities

Department of Molecular and Cellular Biology, Fall 1997, Brown University, Providence, RI. Invited talk: Dynamics in calmodulin crystals

International Union of Crystallography Meeting, August 1996, Seattle, WA. Invited talk on dissertation research

CHESS Journal Club, May 1996, Cornell University, Ithaca, NY. Invited talk on dissertation research

Keck Center for Computational Biology Colloquium, September 1995, Rice University, Houston, TX. Invited talk on dissertation research

DCRT Structural Biology Division, 1994, National Institutes of Health, Bethesda, MD. Invited talk on dissertation research

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Publications in Peer-Reviewed Journals

1. S.M. Gruner, S.L. Barna, M.E. Wall, M.W. Tate, E.F. Eikenberry. 1993. Characterization of polycrystalline phosphors for area x-ray Detectors. Proceedings of the SPIE - The International Society for Optical Engineering 2009:98-108
2. M.W. Tate, E.F. Eikenberry, S.L. Barna, M.E. Wall, J.L. Lowrance, S.M. Gruner. A large-format high-resolution area X-ray detector based on a fiber-optically bonded charge-coupled device (CCD). 1995. Journal of Applied Crystallography 28:196-205
3. R.L. Walter, D.J. Thiel, S.L. Barna, M.W. Tate, M.E. Wall, E.F. Eikenberry, S.M. Gruner and S.E. Ealick. 1995. High-resolution macromolecular structure determination using CCD detectors and synchrotron radiation. Structure 3:835
4. M.E. Wall, S.E. Ealick and S.M. Gruner. 1997. Three-dimensional diffuse X-ray scattering from crystals of *Staphylococcal nuclease*. Proc Natl Acad Sci USA 94:6180-84
5. M.E. Wall, J.B. Clarage and G.N. Phillips, Jr. 1997. Motions of calmodulin characterized using both Bragg and diffuse X-ray scattering. Structure 5:1599-1612
6. M.E. Wall, S. Subramaniam and G.N. Phillips, Jr. 1999. Protein structure determination using a database of interatomic distance probabilities. Protein Sci 8:2720-27.
7. C.S. Tung, M.E. Wall, S.C. Gallagher and J. Trehwella. 2000. A model of troponin-I in complex with troponin-C using hybrid experimental data: the inhibitory region is a β -hairpin. Protein Sci 7:1312-26
8. M.E. Wall, P.A. Dyck and T.S. Brettin. 2001. SVDMAN – singular value decomposition analysis of microarray data. Bioinformatics 6:566-568
9. M.E. Wall, S.H. Francis, J.D. Corbin, K. Grimes, R. Richie-Jannetta, J. Kotera, B.A. Macdonald, R.R. Gibson and J. Trehwella. 2003. Mechanisms associated with cGMP binding and activation of cGMP-dependent protein kinase. Proc Natl Acad Sci USA 100:2380-2385.
10. M.E. Wall, W.S. Hlavacek and M.A. Savageau. 2003. Design principles for regulator gene expression in a repressible gene circuit. J Mol Biol 332:861-876.
11. D. Ming and M.E. Wall. 2005. Quantifying allosteric effects in proteins. Proteins 59:697-707.
12. M.E. Wall, M.J. Dunlop and W.S. Hlavacek. 2005. Multiple functions of a feed-forward-loop gene circuit. J Mol Biol 349:501-514
13. D. Ming and M.E. Wall. 2005. Allostery in a coarse-grained model of protein dynamics. Phys Rev Lett 95:198301
14. D. Ming and M.E. Wall. 2006. Interactions in native binding sites cause a large change in protein dynamics. J Mol Biol 358:213-223
15. D. Ming, M.E. Wall, and K.Y. Sanbonmatsu. 2007. Domain motions of Argonaute, the catalytic engine of RNA interference. BMC Bioinformatics 8:470 (“Highly accessed” designation).
16. D. Ming, M. Anghel, and M.E. Wall. Hidden structure in protein energy landscapes. Phys Rev E. In press.
17. D. Ming, J.D. Cohn, and M.E. Wall. Fast dynamics perturbation analysis for prediction of protein functional sites. BMC Structural Biology. In press.

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Peer-Reviewed Conference Proceedings

18. M.J. Dunlop and M.E. Wall. 2005. Robustness in gene circuits: clustering of functional responses. Proceedings of the 24th American Control Conference 6:4411-4416
19. M.E. Wall. Ligand binding, protein fluctuations, and allosteric free energy. 2006. AIP Conference Proceedings 851:16-33
20. I. Nemenman, G.S. Escola, W.S. Hlavacek, P.J. Unkefer, C.J. Unkefer, M.E. Wall. 2007. Reconstruction of metabolic networks from high-throughput metabolite profiling data: *in silico* analysis of red blood cell metabolism. Ann NY Acad Sci 1115:102-115

Review Articles

21. M.E. Wall, S.C. Gallagher and J. Trehwella. 2000. Large-scale shape changes in proteins and macromolecular complexes. Ann Rev Phys Chem 51:355-80
22. M.E. Wall, W.S. Hlavacek and M.A. Savageau. 2004. Design of gene circuits: lessons from bacteria. Nat Rev Genet 5:34-42.

Book Chapters

23. M.E. Wall, A. Rechtsteiner, L.M. Rocha. 2003. Singular Value Decomposition and Principal Component Analysis. In *A Practical Approach to Microarray Data Analysis*. D.P. Berrar, W. Dubitzky, M. Granzow, eds. pp. 91-109, Kluwer:Norwell, MA.
24. M.E. Wall. Methods and software for diffuse X-ray scattering from protein crystals. Meths Mol Biol. In press.

News Features

25. J.S. Edwards, J.R. Faeder, W.S. Hlavacek, Y. Jiang, I. Nemenman, and M.E. Wall. 2007. q-bio 2007: A Watershed Moment in Modern Biology. Mol Syst Biol 3:148